GAUSSIAN TUTORIAL

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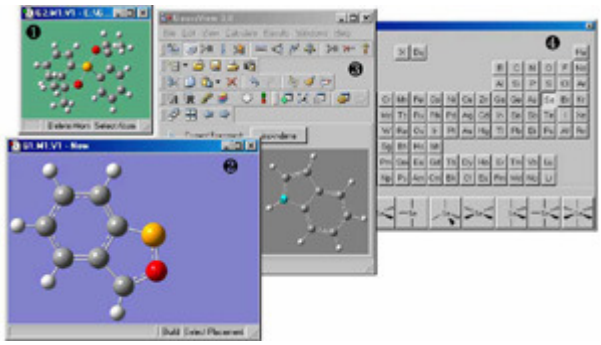
(1) Open Gaussview (version 2.1) on your local machine.
(2) Draw a benzene ring using the builder (already in icon form). Add hydrogens by checking the 'View>Hydrogens' option ((not needed sometimes, but do it all the same). There is an option 'Clean', which uses an MM calculation to do an initial optimization of the geometry very fast.



(3) Optimize geometry: Go to 'Calculate>Gaussian' (Job Type: Optimization, Method: Ground State Mechanics UFF).
(4) Save co-ordinate file using 'Save' - check 'Write Cartesian Coordinates' and give it a name, say benzene.gjf .
(5) Read the output file (benzene.out) to see what it looks like. Re-save it as benzene.gjf
(6) Find dipole moment, nuclear repulsion energy, number of basis functions, number of electrons (alpha and beta, i.e., up and down), and number of primitive gaussians. These are entries in the file.
(7) Now let's run the coordinate file benzene.gjf. Make sure the first line is the Checkpoint line %chk=benzene.chk
(8) Change the next (options) line in benzene.gjf file to the following:
#P lsda/lanl2dz test nosymm
(9) Make sure the syntax of the rest of the file is fine. The next line should be blank, then a title line (write whatever) then a blank, then a line showing charge (0) and spin (2s+1=1 for s=0). Then are the coordinate lines (atomic number, x, y, z) and then finally one blank line in the end.

(10) The overall syntax should look similar to this:

```
%chk=benzene.chk
%mem=6MW
%nproc=1
#P lsda/lanl2dz test nosymm

benzene

0  1
 C                -0.042553    0.000000   -1.446808
 C                -0.042553    0.000000   -0.051648
 C                 1.165198    0.000000    0.645890
 C                 2.373707   -0.001199   -0.051764
 C                 2.373629   -0.001678   -1.446589
 C                 1.165423   -0.000682   -2.144190
 H                -0.994870    0.000450   -1.996567
 H                -0.995066    0.001315    0.497860
 H                 1.165278    0.000634    1.745570
 H                 3.325850   -0.001258    0.498436
 H                 3.325910   -0.002631   -1.996711
 H                 1.165606   -0.000862   -3.243794
```

(11) Submit job from aspen or birch (instructions in Gaussian_PBS.pdf)

(12) The output files created are benzene.out and logfile_benzene, and benzene.chk

(13) From the .out file, read out other info example -- total energy, kinetic, potential and electronic energies, and also eigenenergies (HOMO/LUMO etc). All energies are in Hartrees, so multiply by 27.211. Virtual levels are LUMOs, occupied are HOMOs, Alpha means up spin, and Beta means down spin. Also get Mulliken charges, various multipole moments, etc.

(14) Use the following command:

/itc/apps/gaussian/g98/formchk benzene.chk

This formats the checkpoint file and creates benzene.fchk This gives a lot more info e.g. all the basis sets and their exponents and coefficients, angular moments, forces, etc. which doesn't need to be recomputed again (meaning the next time you run the code with an additional option, you will put in an extra command in your #P line "guess=read" which reads in the checkpoint file and saves on the initial overhead time).

(15) Generate HOMO wave function -- first find level number from the formatted checkpoint file benzene.fchk (number of alpha electrons gives you the HOMO level). Say this is 21 for benzene Then type the following syntax:

/itc/apps/gaussian/g98/cubegen 0 mo=21 benzene.fchk benzene.cub 40 h

This creates a cube-file benzene.cub that has info to plot the 21st (HOMO) molecular orbital

(16) Plot the same from Gaussview - just read in the cube file. (Go to 'Results>Surfaces') Repeat this for PDT. Check HOMO-3 to LUMO+3 energy levels and wave functions for LDA, HF and B3PW91 in LANL2DZ basis set. Compare with the following figure: